

Four component conductance formulation of coherent spin currents

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With recent developments in spintronics, it is now possible to envision “spin-driven” devices with magnets and interconnects that require a new class of transport models using generalized Fermi functions and currents, each with four components: one for charge and three for spin. The corresponding impedance elements are not pure numbers but 4×4 matrices. Starting from the Non-Equilibrium Green’s Function (NEGF) formalism in the elastic, phase-coherent transport regime, we develop spin generalized Landauer-Büttiker formulas involving such 4×4 conductances. In addition to usual “terminal” conductances describing currents at the contacts, we provide “spin-transfer torque” conductances describing the spin currents absorbed by ferromagnetic (FM) regions inside the conductor, specifying both of these currents in terms of Fermi functions at the terminals. These conductances analytically satisfy universal sum rules as well as the spin generalized Onsager’s reciprocity relations and can be represented in a generic 4-component circuit to be used in SPICE-like simulators.

I. INTRODUCTION

The Landauer-Büttiker equation¹ relates the terminal currents I_m to the terminal Fermi functions f_n (FIG. (1))

$$\tilde{I}_m(E) = \frac{1}{q} \sum_n \tilde{G}_{mn}(E) f_n(E) \quad (1a)$$

or to the electrochemical potentials μ_n for linear response

$$I_m = \frac{1}{q} \sum_n G_{mn} \mu_n \quad (1b)$$

These equations have been widely used to describe phase-coherent and elastic transport in conductors and in view of recent developments in the field of spintronics^{2–4}, it is natural to ask whether Eq. (1) can be extended to describe spin currents and spin potentials in phase-coherent conductors.

This can be done by defining (4×1) currents \tilde{I}_m , Fermi functions $f_m(E)$ and potentials μ_m , each having one charge component and three spin components which are related by 4×4 conductance matrices \tilde{G}_{mn} leading to Landauer-Büttiker style expressions of the form:

$$\{\tilde{I}_m(E)\} = \frac{1}{q} \sum_n [\tilde{G}_{mn}(E)] \{f_n(E)\} \quad (2a)$$

or to the electrochemical potentials μ_n for linear response

$$\{I_m\} = \frac{1}{q} \sum_n [G_{mn}] \{\mu_n\} \quad (2b)$$

Conductance matrices of this type could be used in a new class of circuit models with 4-component currents

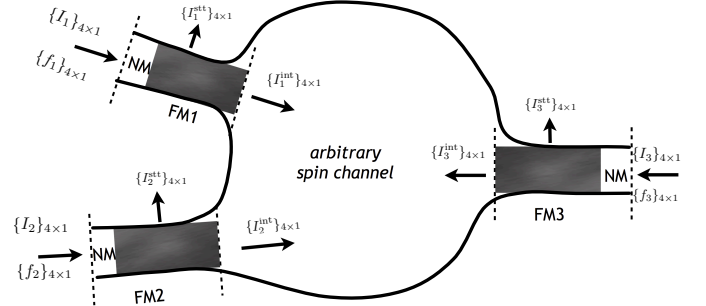


FIG. 1. Schematic of a multi-terminal conductor described by an arbitrary Hamiltonian that could include spin-orbit coupling and/or time-reversal asymmetry. Each terminal ends in a spin-degenerate normal-metal channel that could support both charge and spin potentials and currents, each described by a four-component quantity. The (4×1) terminal current is related to the (4×1) occupation function by a (4×4) terminal conductance matrix, Eq. (2), and to the (4×1) spin-transfer-torque current by the spin-transfer-torque conductance matrix, as shown in Eq. (3).

and potentials that have been used recently to model a limited class of spin logic devices^{5–7}.

In addition to the “terminal” conductance matrix defined by Eq. (2), we also need “spin-transfer-torque” conductances that relate the terminal potentials to the internal currents absorbed within specified surfaces inside the conductor:

$$\{\tilde{I}_m(E)\}^{\text{stt}} = \frac{1}{q} \sum_n [\tilde{G}_{mn}(E)]^{\text{stt}} \{f_n(E)\} \quad (3a)$$

or to the electrochemical potentials μ_n for linear response

$$I_m^{\text{stt}} = \frac{1}{q} \sum_n [G_{mn}]^{\text{stt}} \{\mu_n\} \quad (3b)$$

Typically these could be the difference between interface and terminal currents (FIG. (1), I_m^{int} and I_m respectively)

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representing the spin current absorbed by the FM. This spin-torque current is required as the input to a separate Landau-Lifshitz-Gilbert (LLG) equation which we will not be addressing in this paper.

A recent paper⁸ provided S-matrix based expressions for the terminal conductances of Eq. (2), however the spin-transfer-torque conductances of Eq. (3) have not been addressed before to our knowledge. The main objective of this paper is to provide Non-Equilibrium Green's Function (NEGF)-based expressions for both the terminal and the spin-transfer-torque conductances of Eq. (2) and Eq. (3). In Section(II), we summarize the state-of-the-art standard NEGF formulation⁹⁻²⁰ which provides a benchmark for all our results. Next, we obtain our central results (Section(III)) namely, Eq. (10) for terminal conductances and Eq. (12) for spin-transfer-torque conductances.

In Section(IV and V), we show that Eq. (10) and Eq. (12) automatically satisfy various sum rules and reciprocity relations ensuring charge current conservation, absence of terminal spin currents in equilibrium, and the spin-generalization of Onsager's reciprocity relations, which are all fundamental checks for a theoretically sound transport formalism.

In Section(VI) we provide a generic 4-component circuit representation that can be used to implement terminal and spin-transfer-torque conductances in SPICE-like simulators. Although the circuit components we show are based on our NEGF-based expressions, the 4-component circuit we provide can be used with different 4×4 conductances derived from other microscopic theories, such as Scattering Theory.

Note that the expressions we provide for these conductances are model-independent and could be used in conjunction with any microscopic Hamiltonian, first principles, tight-binding or otherwise, that we may choose to use to describe the conductor.

II. NEGF FORMALISM

Our starting point for the conductances shown in Eq. (2-3) is based on the NEGF(Chapter 8 in²¹ and Chapter 19 in²²) formalism. The main inputs to NEGF (FIG. (2)) are the self-energy functions (Σ) that describe the coupling of the channel to the external contacts, and the Hamiltonian describing the channel itself (H). The two central quantities of interest in NEGF, the retarded Green's function (G^R) and the electron correlation matrix (G^n) are given in terms of these inputs:

$$G^R = [EI - H - \Sigma]^{-1} \quad (4a)$$

$$G^n = G^R \Sigma^{in} G^A \quad (4b)$$

where Σ is the sum of all self-energy matrices, H is the device Hamiltonian, I is the $2N \times 2N$ identity matrix, N being the lattice points of the conductor, E is

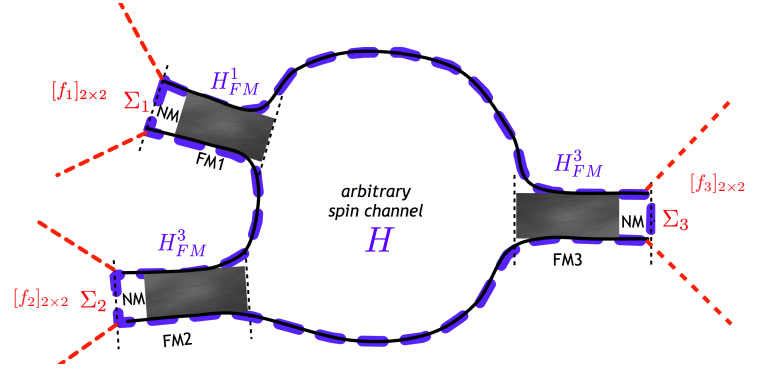


FIG. 2. (Color online) Schematic of the multi-terminal conductor modeled by the NEGF method. Hamiltonian matrix, H , models the shaded region while the self-energy matrices, Σ model the contacts together with 2×2 Fermi functions serving as boundary conditions. The Hamiltonians of the magnetic regions of size $2n \times 2n$ embedded in a zero matrix $2N \times 2N$ are labeled H_{FM}^m are used in the calculation of spin-transfer-torque conductances defined by Eq. (3). Once G^n and G^R are known from Eq. (4a) and Eq. (4b), Eq. (5) can be used to calculate terminal or spin-transfer-torque currents inside the device in the standard NEGF formalism.

energy and G^A is the advanced Green's function, the Hermitian conjugate of the retarded Green's function: $G^A = (G^R)^\dagger$. Σ^{in} appearing in Eq. (4b) is the total 'in-scattering' of electrons that includes the electron injection from the contacts, as well as injection from fictitious contacts due to incoherent scattering mechanisms inside the conductor. We are following the notation used in^{21,22} with $G^n \equiv -iG^<$ and $\Sigma^{in} = -i\Sigma^<$.

Once the Green's function (Eq. (4a)) and the electron correlation matrix (Eq. (4b)) are known, the net flux of spins entering into the conductor volume (Ω) can be expressed by tracing the NEGF current operator with Pauli spin matrices^{21,22}:

$$\text{tr.}[S_\alpha I_{op}] = \frac{q}{h} \text{tr.} \left[i S_\alpha \begin{pmatrix} G^n H - H G^{n+} \\ G^n \Sigma^\dagger - \Sigma G^{n+} \\ G^R \Sigma^{in} - \Sigma^{in} G^A \end{pmatrix} \right] \quad (5)$$

where Σ and Σ^{in} represent the total self-energy and total in-scattering matrices, summed over all contacts and S_α , an "expanded" Pauli spin matrix such that $S_\alpha = I \otimes \sigma_\alpha$, I being the $N \times N$ identity matrix (N : number of lattice points) and σ_α is the 2×2 Pauli spin matrix for a spin direction α , and $I_{2 \times 2}$ for charge.

Eq. (5) is widely used in the literature to calculate currents through conventional spin-torque devices, such as MTJs⁹⁻¹⁸, and through sophisticated spin-devices^{19,20} for both terminal spin currents, and for internal spin currents involving spin-transfer-torque calculations. Therefore, the main benchmark for our results (Eq. (10)-Eq. (12)) has been to make extensive numerical comparisons with Eq. (5), using random Hamiltonians representing arbitrary spin channels to ensure the validity of

our expressions presented in the next section.

III. DERIVATION OF CENTRAL RESULTS

Any of the NEGF matrices defined in Eq. (4) can be specified as a Kronecker product of a real space matrix (of size $N \times N$) and a spin space component (of size 2×2). For example, the “broadening matrix” due to non-magnetic contact m can be written as:

$$\Gamma_m = i(\Sigma_m - \Sigma_m^\dagger) = \gamma_m \otimes I_{2 \times 2} \quad (6a)$$

where γ_m is the $N \times N$ real space component of the full broadening matrix, and it is the anti-Hermitian part of the self-energy matrix Σ_m .

When the contacts are driven out of equilibrium by external sources, the inscattering function has to be modified through its spin component:

$$\Sigma_m^{in} = \gamma_m \otimes \left(f_m^c I + \vec{f}_m^s \cdot \vec{\sigma} \right) \quad (6b)$$

Where $(f_m^c I + \vec{f}_m^s \cdot \vec{\sigma})$ is the 2×2 matrix specifying the occupation probabilities of spin and charge components at a given contact which reduces to $f_m^c I$ for ordinary charge-driven transport.

Next, we observe that the current operator of Eq. (5) is zero at steady state since it represents a) the sum of all the inflow through the contact boundaries and b) the “recombination/generation (R/G)” currents within the conductor volume. The R/G currents are ordinarily zero for charge currents, however, may exist for spin-currents due to magnetic fields or spin-orbit coupling within the conductor (FIG. 3).

In Appendix C, we show that the total influx for a given spin direction α (Eq. (5)) can be mathematically decomposed into these two distinct components, the first being the spin-current injected by contact m :

$$I_m^\alpha = \frac{q}{h} \text{tr.} \left(i S_\alpha \left[G^n \Sigma_m^\dagger - \Sigma_m G^n \right] + i S_\alpha \left[G^R \Sigma_m^{in} - \Sigma_m^{in} G^A \right] \right) \quad (7)$$

And the second component being the generation of spin currents within the conductor volume:

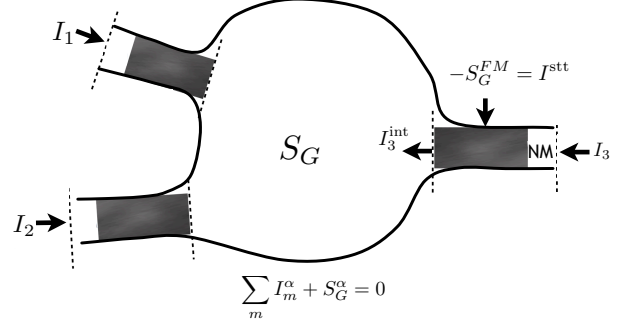
$$S_G^\alpha = \frac{q}{h} \text{tr.} [i S_\alpha (H G^n - G^n H)] \quad (8)$$

so that Eq. (5) can be written as:

$$\text{tr.} [S_\alpha I_{op}] = \sum_m I_m^\alpha + S_G^\alpha = 0 \quad (9)$$

Terminal Conductances: Defining the terminal conductances as:

$$[\tilde{G}_{mn}]^{\alpha\beta} = \frac{1}{q} \frac{\partial I_m^\alpha}{\partial f_n^\beta}$$



$$I_m^\alpha = \frac{q}{h} i \text{tr.} \left(\begin{array}{l} S_\alpha [G^n \Sigma_m^\dagger - \Sigma_m G^n] \\ + S_\alpha [G^R \Sigma_m^{in} - \Sigma_m^{in} G^A] \end{array} \right) \quad S_G^\alpha = \frac{q}{h} i \text{tr.} [S_\alpha H G^n - S_\alpha G^n H]$$

FIG. 3. NEGF current operator (Eq. (5)) can be decomposed into the total inflow from contacts and the recombination-generation of spin currents inside the conductor. The spin-transfer-torque is a subset of this total recombination, since it is restricted within the FM regions.

substituting Eq. (4b) and Eq. (6b) in Eq. (7) the conductances can be expressed as:

$$[\tilde{G}_{mn}]^{\alpha\beta} = \frac{q^2}{h} \text{tr.} \left[S_\alpha \left(\begin{array}{l} G^R \Gamma_n S_\beta G^A \Sigma_m^\dagger \\ - \Sigma_m G^R \Gamma_n S_\beta G^A \end{array} \right) + S_\alpha (i [G^R \Gamma_m S_\beta - \Gamma_m S_\beta G^A]) \delta_{mn} \right]$$

Since the contacts are assumed to be non-magnetic, self-energy Σ and broadening matrices Γ commute with the spin matrices $S_{\alpha,\beta}$, allowing the use of Eq. (6a) to simplify further:

$$[\tilde{G}_{mn}]^{\alpha\beta} = \frac{q^2}{h} \text{tr.} \left[i \left(\begin{array}{l} S_\beta S_\alpha G^R \Gamma_m \\ - S_\alpha S_\beta G^A \Gamma_m \end{array} \right) \delta_{mn} \right] - \text{tr.} [S_\alpha \Gamma_m G^R S_\beta \Gamma_n G^A] \quad (10)$$

which is the central result for terminal conductances defined in Eq. (2).

Spin-transfer-torque Conductances: The spin-transfer-torque absorbed by the FM regions inside the channel are quantified by the negative “generation” rate within these volumes:

$$-S_G^{FM} = \frac{q}{h} \text{tr.} [i S_\alpha (H_{FM}^m G^n - G^n H_{FM}^m)] \quad (11)$$

where H_{FM}^m is the $2n \times 2n$ Hamiltonian matrix of the ferromagnetic layer (for a magnet with n physical points), embedded in a $2N \times 2N$ zero matrix. This current can then be used to define spin-transfer-torque conductances that provide the spin-torque absorbed by the FM:

$$[\tilde{G}_{mn}]^{\text{stt}-\alpha\beta} = \frac{1}{q} \frac{\partial (-S_G^{FM})}{\partial f_n^\beta}$$

so that

$$\left[\tilde{G}_{mn}\right]^{\text{stt}-\alpha\beta} = \frac{q^2}{h} \text{tr.} \left[i \begin{pmatrix} H_{FM}^m S_\alpha \\ -S_\alpha H_{FM}^m \end{pmatrix} G^R S_\beta \Gamma_n G^A \right] \quad (12)$$

where we have substituted Eq. (4b) in Eq. (11) to obtain our central result for $\left[\tilde{G}_{mn}\right]^{\text{stt}}$ defined in Eq. (3). We also note that Eq. (12) is general and can be used within any closed surface within the device, such as magnets that are situated in the middle of the device as well as those situated by the contacts.

Reducing to the Charge Limit: The standard result for pure charge conductance is a subset of the terminal conductance matrix shown in Eq. (10), and can simply be obtained by using I in place of S_α and S_β :

$$\left[\tilde{G}_{mn}\right]^{cc} = \frac{q^2}{h} \text{tr.} (\Gamma_m A \delta_{mn} - \Gamma_m G^R \Gamma_n G^A) \quad (13)$$

where we have made use of the NEGF identity:

$$A = i [G^R - G^A] \quad (14)$$

A being the ‘spectral density’ matrix per unit energy.

Note that the second term in Eq. (13) picks up Pauli spin matrices for the two spin indices (S_α, S_β) to become the second term of Eq. (10) while the first terms are fundamentally different: Because different spin-directions do not commute in general, S_α and S_β of the first term of Eq. (10) cannot be exchanged to use Eq. (14) in Eq. (13). Therefore, Eq. (13) cannot be generalized trivially in conjunction with Pauli spin matrices, $S_{\alpha,\beta}$ to obtain Eq. (10) without starting from the proper current operator of Eq. (5).

IV. SUM RULES

In this section, starting from Eq. (10 and 12) we show universal sum rules that the proposed conductance expressions analytically satisfy. We start with the general multi-terminal conductance matrix relating currents and occupation functions at different terminals:

$$\begin{bmatrix} I^c \\ I^z \\ I^x \\ I^y \end{bmatrix} = \begin{matrix} c & z & x & y \\ \begin{pmatrix} \tilde{G}^{cc} & \tilde{G}^{cz} & \tilde{G}^{cx} & \tilde{G}^{cy} \\ \tilde{G}^{zc} & \tilde{G}^{zz} & \tilde{G}^{zx} & \tilde{G}^{zy} \\ \tilde{G}^{xc} & \tilde{G}^{xz} & \tilde{G}^{xx} & \tilde{G}^{xy} \\ \tilde{G}^{yc} & \tilde{G}^{yz} & \tilde{G}^{yx} & \tilde{G}^{yy} \end{pmatrix} \end{matrix} \begin{bmatrix} f^c \\ f^z \\ f^x \\ f^y \end{bmatrix}$$

where each entry in the conductance matrix is a $P \times P$ matrix while the currents $I^{c,s}$ and occupation functions $f^{c,s}$ are $P \times 1$ column vectors, P being the number of terminals in the conductor; so that the submatrix \tilde{G}^{cc} can be identified as the conductance matrix describing the coherent charge currents.

Charge Conservation (Terminal): Regardless

of how charge currents are generated through \tilde{G}^{cc} or \tilde{G}^{cs} , charge conservation requires them to add up to zero at steady state, in both linear response and high-bias regimes. This requires two universal sum rules to hold:

$$\sum_{m=1}^P \left[\tilde{G}_{mn}\right]^{cc} = 0 \quad (15a)$$

which is a well-known sum rule in the context of pure charge currents. For spin-generated charge currents we find a similar sum rule:

$$\sum_{m=1}^P \left[\tilde{G}_{mn}\right]^{cs} = 0 \quad (15b)$$

We show in Appendix A that both these equations are analytically satisfied by the conductance matrices of Eq. (10).

Equilibrium Currents (Terminal): In equilibrium, there are no spin accumulations in the contacts since they are assumed to be non-magnetic, making all occupation functions have the form:

$$f_{eq} = [f_0 \ 0 \ 0 \ 0]^T$$

at a given energy. Because no net charge current can flow through the terminals in equilibrium:

$$\sum_{n=1}^P \left[\tilde{G}_{mn}\right]^{cc} = 0 \quad (16a)$$

The fact that no net spin current can flow through the terminals in equilibrium requires:

$$\sum_{n=1}^P \left[\tilde{G}_{mn}\right]^{sc} = 0 \quad (16b)$$

This once debated result (See²³ and references therein) was established from Scattering Theory in the context of spin-orbit coupling for devices with non-magnetic leads. In Appendix A we prove this result analytically starting from Eq. (10) and observe that having magnets or magnetic fields (in addition to any spin-orbit interaction) inside the conductor does not change this basic conclusion. We also note that there are no general sum rules for the spin to spin conductances $\left[\tilde{G}_{mn}\right]^{ss}$.

Charge Conservation (Spin-transfer-torque): Since no charge currents can be generated or absorbed within the FM regions, the generation term S_G becomes identically zero (by choosing $S_\alpha = I$ in Eq. (12)) requiring:

$$\left[\tilde{G}_{mn}\right]^{\text{stt}-cc} = 0 \quad (17a)$$

for all (m,n). Also:

$$\left[\tilde{G}_{mn}\right]^{\text{stt}-cs} = 0 \quad (17b)$$

Equilibrium Currents (Spin-transfer-torque): Under equilibrium conditions, the spin-torque applied to the ferromagnetic layer does not necessarily vanish, unlike terminal equilibrium currents:

$$\sum_n [\tilde{G}_{mn}]^{\text{stt-sc}} \neq 0$$

suggesting interesting practical possibilities due to spin currents exerting spin-torque under zero bias conditions.

V. RECIPROCITY

In this section, starting from time-reversibility conditions for Green's functions we show that the terminal conductances (Eq. 10) satisfy the spin-generalization of Onsager's reciprocity in linear response conditions (a result discussed in detail in⁸):

$$\left[\tilde{G}_{mn} \right]^{\alpha\beta} \Big|_{+B} = \left[\tilde{G}_{nm} \right]^{\beta\alpha} \Big|_{-B} (-1)^{n_\alpha + n_\beta} \quad (18)$$

where the exponents n_α and n_β are 0 for charge and 1 for spin indices, respectively. Physically, Eq. (18) can be justified by noting that reversing time causes spin-currents and spin-voltages to change sign, while charge currents and charge voltages remain invariant²⁴, requiring the $n_{\alpha,\beta}$ factors in Eq. (18). To show that our conductances satisfy Eq. (18), we first observe that time-reversibility conditions for Green's functions requires:

$$G^R|_{+B} = S_y (G^R)^T S_y|_{-B} \quad (19)$$

where G^R is the retarded Green's function matrix, S_y is the expanded Pauli spin matrix in the y-direction while T denotes matrix transpose. In Appendix B, we start from Eq. (10) and Eq. (19) to prove Eq. (18).

The spin-transfer-torque conductances are not related to one another with universal reciprocity relations, because the currents and occupations functions are defined at different cross-sections.

VI. CIRCUIT REPRESENTATION

FIG. (4) shows a possible circuit representation of the terminal conductance matrices that can be readily implemented in SPICE-like circuit simulators. The example is a 2-Terminal structure for simplicity; however, a similar circuit can be implemented for a conductor with any number of terminals. The circuit components that are shown in FIG. (4) are all uniquely defined in terms of the terminal conductances:

$$\begin{aligned} gs_1 &= \tilde{G}_{11} + \tilde{G}_{21} & gs_2 &= \tilde{G}_{22} + \tilde{G}_{12} \\ g &= -(\tilde{G}_{12} + \tilde{G}_{21})/2 & \beta &= g^{-1}(\tilde{G}_{21} - \tilde{G}_{12})/2 \end{aligned} \quad (20)$$

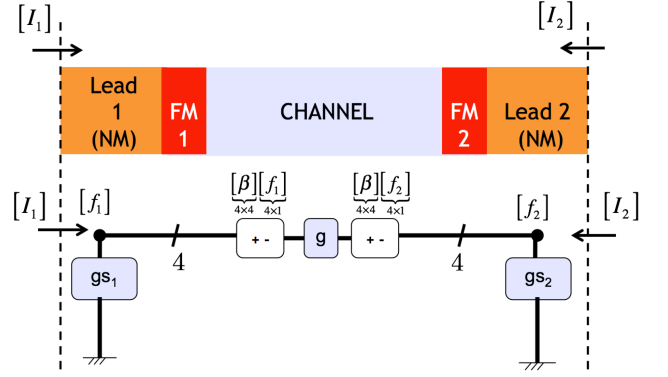


FIG. 4. (Color online) Four component circuit representation of a 2-Terminal spin device with an arbitrary channel, and magnetic contacts. All nodes carry 4 currents and 4 voltages, while all circuit elements are 4×4 matrices, uniquely defined in terms of conductances shown in Eq. (10).

making each of these conductances are 4×4 matrices. The following circuit equations can be used to arrive at Eq. (20):

$$I_1 = gs_1 f_1 + g [(I - \beta) f_1 - (I + \beta) f_2] \quad (21)$$

$$I_2 = gs_2 f_2 + g [(I + \beta) f_2 - (I - \beta) f_1] \quad (22)$$

The circuit elements here are such that all currents and voltages are specified at a given energy. In linear response however, the conductance elements in FIG. (4) can be summed over a given energy range to represent full I-V characteristics with a single circuit in terms of currents and voltages. Note that the circuit elements defined in Eq. (20) are generic and can be used with 4-component conductances based on other microscopic theories, such as Scattering Theory.

There are two different features of the circuit shown in FIG. (4) compared to ordinary charge-based circuits: a) Shunt conductances, a consequence of recombination (generation) of spin-currents within the conductor and b) Voltage Controlled Voltage Sources (VCVS), a consequence of a possible non-reciprocity of the general network.

The shunt conductances gs_1 and gs_2 account for differences in spin currents entering and leaving the device whose cc and cs elements are zero, prohibiting charge currents through these conductances. The VCVS elements are required since a physically asymmetric device having a $+z$ magnet on the left and a $+x$ magnet on the right, will “look” different to an incoming spin current from both sides. Note that in the limit of pure charge-based networks, 2-Terminal devices are reciprocal even in the presence of magnetic fields, whereas for spin-based networks 2-Terminal devices may show non-reciprocity even without magnetic fields but in the presence of spin-orbit interactions. Similar VCVS elements have been used to describe non-reciprocal circuits of the classical Hall Effect for possible circuit implementations²⁵.

For self-consistent magnetization dynamics and transport simulations, the same circuit implementation can be used with spin-transfer-torque conductances that would be supplied to an LLG solver in a SPICE implementation.

VII. SUMMARY

Existing NEGF-based models for charge-based nanoelectronic devices often the conductance expression, $G^{cc} = \frac{q^2}{h} \text{tr.} [\Gamma_1 G^R \Gamma_2 G^A]$ in the elastic, coherent transport regime. On the other hand, recent advances in spintronics have raised the possibility of spin potential-driven electronic devices. This paper provides conductance expressions involving spin potentials and spin currents generalizing the charge conductance G^{cc} of NEGF-based models. In addition to terminal conductances, we provide “spin-transfer-torque” conductances to be used in self-consistent simulations of magnetization dynamics and spin transport. We have shown that these conductances pass critical tests by automatically satisfying universal sum rules and reciprocity relations that must hold irrespective of the details of transport. Finally, we have represented our results in a generic 4-component circuit which can be used separately by 4-component conductances of other origins, to be implemented in SPICE-like simulators towards a unified description of hybrid devices involving existing CMOS and spintronic circuit elements.

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Appendix A

Objective: In this Appendix, we prove Eq. (15a,15b,16a,16b) starting from Eq. (10).

$$\sum_{m=1}^P [\tilde{G}_{mn}]^{cc} = 0$$

Starting from Eq. (10) for cc elements:

$$\sum_m [\tilde{G}_{mn}]^{cc} = \frac{q^2}{h} \sum_m \begin{pmatrix} i \text{tr.} [\Gamma_m G^R - \Gamma_m G^A] \delta_{mn} \\ -\text{tr.} [\Gamma_m G^R \Gamma_n G^A] \end{pmatrix}$$

And using the following NEGF identities:

$$A = i [G^R - G^A] = \sum_k G^R \Gamma_k G^A = \sum_k G^A \Gamma_k G^R$$

The desired sum rule then, follows:

$$\sum_m [\tilde{G}_{mn}]^{cc} = \frac{q^2}{h} \begin{pmatrix} \text{tr.} [\Gamma_n A] \\ -\text{tr.} \left[G^A \sum_m \underbrace{\Gamma_m G^R \Gamma_n}_A \right] \end{pmatrix} = 0$$

$$\sum_{m=1}^P [\tilde{G}_{mn}]^{cs} = 0$$

Specializing to cs elements (s representing spin indices x, y, z):

$$\sum_m [\tilde{G}_{mn}]^{cs} = \frac{q^2}{h} \sum_n \begin{pmatrix} i \text{tr.} [S_\beta \Gamma_m G^R - S_\beta \Gamma_m G^A] \delta_{mn} \\ -\text{tr.} [\Gamma_m G^R S_\beta \Gamma_n G^A] \end{pmatrix}$$

using the same NEGF identities, we obtain:

$$\sum_m [\tilde{G}_{mn}]^{cs} = \frac{q^2}{h} \begin{pmatrix} \text{tr.} [S_\beta \Gamma_n A] \\ -\text{tr.} \left[G^A \sum_m \underbrace{\Gamma_m G^R S_\beta \Gamma_n}_A \right] \end{pmatrix} = 0$$

$$\sum_{n=1}^P [\tilde{G}_{mn}]^{cc} = 0$$

Starting from Eq. (10) for cc :

$$\sum_n [\tilde{G}_{mn}]^{cc} = \frac{q^2}{h} \sum_n \begin{pmatrix} i \text{tr.} [\Gamma_m G^R - \Gamma_m G^A] \delta_{mn} \\ -\text{tr.} [\Gamma_m G^R \Gamma_n G^A] \end{pmatrix}$$

Making use of the NEGF identities shown above:

$$\sum_n [\tilde{G}_{mn}]^{cc} = \frac{q^2}{h} \begin{pmatrix} \text{tr.} [\Gamma_m A] \\ -\text{tr.} \left[\Gamma_m G^R \sum_n \underbrace{\Gamma_n G^A}_A \right] \end{pmatrix} = 0$$

$$\sum_{n=1}^P [\tilde{G}_{mn}]^{sc} = 0$$

Specializing to sc elements for the conductance matrices:

$$\sum_n [\tilde{G}_{mn}]^{sc} = \frac{q^2}{h} \sum_n \begin{pmatrix} i \text{tr.} [S_\alpha \Gamma_m G^R - S_\alpha \Gamma_m G^A] \delta_{mn} \\ -\text{tr.} [S_\alpha \Gamma_m G^R \Gamma_n G^A] \end{pmatrix}$$

we have:

$$\sum_n [\tilde{G}_{mn}]^{sc} = \frac{q^2}{h} \begin{pmatrix} \text{tr.} [S_\alpha \Gamma_m A] - \\ \text{tr.} \left[S_\alpha \Gamma_m \sum_n \underbrace{G^R \Gamma_n G^A}_A \right] \end{pmatrix} = 0$$

Appendix B

Objective: In this Appendix, we start from Eq. (10) to prove Eq. (18)

$$[\tilde{G}_{mn}]^{\alpha\beta} \Big|_{+B} = \frac{q^2}{h} \begin{pmatrix} \text{tr.} [i S_\beta S_\alpha \Gamma_m G^R - S_\alpha S_\beta \Gamma_m G^A] \delta_{mn} \\ -\text{tr.} [S_\alpha \Gamma_m G^R S_\beta \Gamma_n G^A] \end{pmatrix}_{+B}$$

and write the equivalent expression for B using the time-reversibility rules for Green's functions (Eq. (19) in the text):

$$= \frac{q^2}{h} \begin{pmatrix} -\text{tr.} \left[S_\alpha (\Gamma_m)^T \left(S_y (G^R)^T S_y \right) S_\beta (\Gamma_n)^T \left(S_y (G^A)^T S_y \right) \right] + \\ i \text{ tr.} \left[\begin{array}{cc} S_\beta S_\alpha (\Gamma_m)^T \left(S_y (G^R)^T S_y \right) - & \\ S_\alpha S_\beta (\Gamma_m)^T \left(S_y (G^A)^T S_y \right) & \end{array} \right] \delta_{mn} \end{pmatrix}_{-B}$$

Note that the broadening matrices Γ only pick up a transpose under time reversal because they correspond to non-magnetic contacts with no spin preference. First we ob-

serve:

$$S_y S_\alpha = (S_\alpha)^T S_y (-1)^{n_\alpha}$$

where α is a spin or charge index, and n_α is 1 for spin indices and 0 for charge. Next, using the cyclic property of traces with the fact that Γ commutes with Pauli matrices (non-magnetic contacts):

$$= \frac{q^2}{h} \begin{pmatrix} -\text{tr.} \left[\underbrace{S_y S_\alpha S_y}_{S_\alpha^T (-1)^{n_\alpha}} (\Gamma_m)^T (G^R)^T \underbrace{S_y S_\beta S_y}_{S_\beta^T (-1)^{n_\beta}} (\Gamma_n)^T (G^A)^T \right] + \\ i \text{ tr.} \left[\begin{array}{cc} \underbrace{S_y S_\beta S_\alpha S_y}_{S_\beta^T S_\alpha^T (-1)^{(n_\alpha + n_\beta)}} & (\Gamma_m)^T (G^R)^T - \\ \underbrace{S_y S_\alpha S_\beta S_y}_{S_\alpha^T S_\beta^T (-1)^{(n_\alpha + n_\beta)}} & (\Gamma_m)^T (G^A)^T \end{array} \right] \delta_{mn} \end{pmatrix}_{-B}$$

simplifying to:

$$= \frac{q^2}{h} \begin{pmatrix} -\text{tr.} \left[(S_\beta \Gamma_n G^R S_\alpha \Gamma_m G^A)^T \right] (-1)^{n_\alpha + n_\beta} + \\ i \text{ tr.} \left[(G^R \Gamma_m S_\alpha S_\beta - G^A \Gamma_m S_\beta S_\alpha)^T \right] \delta_{mn} (-1)^{(n_\alpha + n_\beta)} \end{pmatrix}_{-B}$$

the right hand side is by definition defined as:

$$[G_{mn}]^{\alpha\beta} \Big|_{+B} = [G_{nm}]^{\beta\alpha} \Big|_{-B} (-1)^{n_\alpha + n_\beta}$$

since trace of A^T is equal to trace A, proving the reciprocity relation shown in the main text.

Appendix C

Objective: In this Appendix, we start from Eq. (5) and show that it can be decomposed into the sum of two distinct components, Eq. (7) and Eq. (8). Starting from:

$$\text{tr.} [S_\alpha I_{op}] = \frac{q}{h} \text{tr.} \left[i S_\alpha \begin{pmatrix} G^n H - H G^n + \\ G^n \Sigma^\dagger - \Sigma G^n + \\ G^R \Sigma^{in} - \Sigma^{in} G^A \end{pmatrix} \right] \quad (\text{C1})$$

Using the cyclic property of trace operator:

$$\begin{aligned} & \text{tr.} [i (HS_\alpha - S_\alpha H) G^n] + \\ & \text{tr.} [i (\Sigma^\dagger S_\alpha - S_\alpha \Sigma) G^n] + \\ & \text{tr.} [i (S_\alpha G^R - G^A S_\alpha) \Sigma^{in}] \end{aligned}$$

In explicit notation where (m, n) refer to lattice sites where each A_{mn} below corresponds to a 2×2 spin matrix:

$$\begin{aligned} & \sum_{n,m} [i (HS_\alpha - S_\alpha H)_{n,m} (G^n)_{m,n}] + \\ & \sum_{n,m} [i (\Sigma^\dagger S_\alpha - S_\alpha \Sigma)_{n,m} (G^n)_{m,n}] + \\ & \sum_{n,m} [i (S_\alpha G^R - G^A S_\alpha)_{n,m} (\Sigma^{in})_{m,n}] \end{aligned}$$

First Term: The first coefficient in the first term reads:

$$\begin{aligned} & i (HS_\alpha - S_\alpha H)_{n,m} \\ & = \sum_k H_{n,k} (S_\alpha)_{k,m} - (S_\alpha)_{n,k} H_{k,m} \\ & = H_{n,m} (S_\alpha)_{m,m} - (S_\alpha)_{n,n} (H)_{n,m} \\ & = H_{n,m} \sigma - \sigma H_{n,m} \end{aligned}$$

Inside the non-magnetic contacts, $H_{n,m}$ commutes with

all Pauli spin matrices for $(m, n) \in$ contact boundaries, making this term identically zero along all contact regions.

Second Term: The first coefficient in the second term of reads:

$$\begin{aligned} & (\Sigma^\dagger S_\alpha - S_\alpha \Sigma)_{n,m} \\ & = \sum_k \Sigma_{n,k}^\dagger (S_\alpha)_{k,m} - (S_\alpha)_{n,k} \Sigma_{k,m} \\ & = \Sigma_{n,m}^\dagger (S_\alpha)_{m,m} - (S_\alpha)_{n,n} \Sigma_{n,m} \\ & = \Sigma_{n,m}^\dagger \sigma - \sigma \Sigma_{n,m} \end{aligned}$$

The term $\Sigma_{n,m}^\dagger$ is zero unless (m, n) are lattice points within contact boundaries, making the second term non-zero, only along contact regions.

Third Term: The third term will be zero unless $\Sigma_{m,n}^{in}$ is non-zero. By definition:

$$\Sigma^{in} = \gamma \otimes [f]_{2 \times 2}$$

where γ is the $N \times N$ broadening matrix, N being the number of lattice points while $\gamma_{m,n}$ is non-zero only for (m, n) that are lattice points within contact boundaries. In summary, second and third term can be associated with Eq. (7) and the first term with Eq. (8).